CONTENTS OF VOLUME 2

NUMBER 1

ORIGINAL RESEARCH ARTICLES

Chance Classifications by Non-parametric Linear Discriminant Functions
B. K. Lavine, P. C. Jurs and D. R. Henry 1

Identification and Substructure Analysis of Oligosaccharide Chains Derived from Glycoproteins by Computer Retrieval of High-resolution ^{1}H-NMR Spectra
D. S. M. Bot, P. Cleij, H. A. van't Klooster, H. van Halbeek, G. A. Veldink and J. F. G. Vliegenthart 11

Taxonomy Based on Chemical Constitution: Differentiation of Africanized Honey-bees from European Honey-bees
B. K. Lavine, D. A. Carlson, D. Henry and P. C. Jurs 29

Selection of Optimal Regression Models Via Cross-validation
D. W. Osten 39

Expert System for Knowledge-based Modelling of Analytical Laboratories as a Tool for Laboratory Management
J. Klaessens, T. Saris, B. Vandeginste and G. Kateman 49

The Effect of Interferences and Calibration Design on Accuracy: Implications for Sensor and Sample Selection
A. Lorber and B. R. Kowalski 67

SHORT COMMUNICATIONS

Principal Component Variable Discriminant Plots: a Novel Approach for Interpretation and Analysis of Multi-class Data
N. B. Vogt 81

Monte Carlo Studies of Non-parametric Linear Discriminant Functions
B. K. Lavine and D. R. Henry 85

Announcements and Call for Papers 91

NUMBER 2

ORIGINAL RESEARCH ARTICLES

Estimation of Prediction Error for Multivariate Calibration
A. Lorber and B. R. Kowalski 93

The Application of Submatrix Analysis to Disordered Spectroscopic Data
H. M. Cartwright and H. A. Farley 111

A Method for Detecting Potentially Unreliable Estimates when Using the Burdick/Rayens Model for Estimating Linear Mixing Proportions
W. S. Rayens 121

Estimation of Second-order Chemical Kinetic Parameters by Using Information-based Extended Kalman Filtering
T. Q. Barker and S. D. Brown 137

Principal Component Regression in NIR Analysis: Viewpoints, Background Details and Selection of Components
T. Næs and H. Martens 155

Book Review 169; Announcement 170

NUMBER 3

ORIGINAL RESEARCH ARTICLES

PLS Assessment of the Performance of Short-term Tests for Carcinogens
M. L. Tosato, D. Cesareo, L. Passerini and S. Clementi 171

Evaluation of Computing Capabilities of a Hierarchy of Mini-to-Supercomputers: Applications to Ion Microscopic Analysis
Y.-C. Ling, D. N. Bernardo and G. H. Morrison 189

Savitzky–Golay Filtering in Particle Characterization
S. M. Wolfrum and N. J. A. van Veen 203

PLS Regression Methods
A. Höskuldsson 211

Book Review 229; News from the International Chemometrics Society 230

NUMBER 4

REVIEW ARTICLE

Notes on the History and Nature of Partial Least Squares (PLS) Modelling
P. Geladi 231

ORIGINAL RESEARCH ARTICLES

Tensorial Calibration: I. First-order Calibration
E. Sanchez and B. R. Kowalski 247

Tensorial Calibration: II. Second-order Calibration
E. Sanchez and B. R. Kowalski 265

Source Contributions to Ambient Aerosol Calculated by Discriminant Partial Least Squares Regression (PLS)
R. Vong, P. Geladi, S. Wold and K. Esbensen 281

Special Issue Review 297: Book Reviews 298; Author Index 300; Key Word Index 301